Magnetic edge states in spin triplet superconductors

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We show that a spontaneous magnetic moment may appear at the edge of a spin-triplet superconductor if the system allows for pairing in a subdominant channel. To unveil the microscopic mechanism behind such effect we combine numerical solution of the Bogoliubov-De Gennes equations for a tight-binding model with nearest-neighbor attraction, and the symmetry based Ginzburg-Landau approach. We find that a potential barrier modulating the electronic density near the edge of the system leads to a non-unitary superconducting state close to the boundary where spin-singlet pairing coexists with the dominant triplet superconducting order. We demonstrate that the spin polarization at the edge appears due to the inhomogeneity of the non-unitary state and is manifested via lifting of the spin-degeneracy of the Andreev bound-states.

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Introduction. Recognition that the surface states in correlated materials reflect the nature of the interactions and orders existing in the bulk has led to a very significant research effort aimed at the understanding, and potential control, of these electronic states [1–3]. Systems where the bulk of the material is gapped but the boundary supports gapless modes are especially interesting since under these conditions the surface states are robust, and may be topologically protected, i.e. their existence relies on the global symmetries of the bulk state and does not depend on the details of the surface scattering and other sample-dependent parameters [2]. The bulk gap may be due to the band structure, or, in a metal, may arise at low temperatures from electron-electron interaction, as in superconductors [4]. Simple band insulators or conventional superconductors do not support robust low-energy states at the boundary, but it is the study of their counterparts with the bulk that is topologically non-trivial, and hence the bulk-boundary correspondence theorem dictates the existence of the surface states, that has been a focus of much recent attention [1, 2, 4].

One of the best candidates for the topological superconductivity is Sr_2RuO_4, where the emergent consensus indicates triplet chiral pairing, with time-reversal symmetry broken by the orbital degrees of freedom [5]. In this material the topologically protected edge states have been predicted, and their signatures were recently found in tunnelling spectroscopy [6]. The quasiparticles reflecting off the sample boundary experience the sign change of the superconducting order parameter along their trajectory, which gives rise to so-called Andreev bound states (ABS) near the surface. Emergence of ABS has been well investigated in high-T_c cuprates and a number of other unconventional superconductors [4, 7, 8].

In this Letter we investigate the nature of the Andreev bound states at the surface of spin triplet superconductors. We perform a microscopic self-consistent calculation, including the realistic surface barrier of a finite width and height and the possibility of pairing in one or more subdominant channels [7]. We find that a) a subdominant *in-phase* s-wave superconducting order exists near the edge of the sample; b) the in-phase s-wave component gives a non-unitary superconducting state at the boundary; c) as a result, the ABS is spin-polarized, leading to a finite surface magnetization. We analyze the conditions for the existence of the magnetic surface states, and we investigate their spectrum. These numerical results are confirmed by carrying out a Ginzburg-Landau expansion of the free energy. Our work strongly suggests that triplet superconductors can be used in spin-active heterostructures.

Model and formalism. We consider a two-dimensional superconductor in a slab geometry with two parallel interfaces separating it from the vacuum. Denoting by x and y the directions perpendicular and parallel to the interfaces, respectively, we assume that the system is uniform along the y axis, so that the translational symmetry is broken only in the x direction. The Hamiltonian is then defined on a square lattice of size $L \times L$ (we set the lattice constant to unity), with periodic boundary conditions along y,

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} (c^{\dagger}_{\mathbf{i}\,\sigma} c_{\mathbf{j}\,\sigma} + \text{h.c.}) - \mu \sum_{\mathbf{i},\sigma} n_{\mathbf{i}\sigma} - \sum_{\langle \mathbf{i},\mathbf{j}\rangle} V\,(n_{\mathbf{i}\uparrow} n_{\mathbf{j}\downarrow} + n_{\mathbf{i}\downarrow} n_{\mathbf{j}\uparrow}) + \sum_{\mathbf{i}} U(i_x) n_{\mathbf{i}\sigma}\,. \quad (1)$$

Here the lattice sites are labelled by $\mathbf{i} \equiv (i_x, i_y)$, with i_x and i_y integers between 0 and L, $\langle \mathbf{i},\mathbf{j}\rangle$ denote nearest-neighbor sites, and μ is the chemical potential. The nearest-neighbor attractive interaction $-V$ ($V > 0$) is effective in both singlet and triplet pairing channels. All the energies are in units of the hopping parameter t. The two parallel edges of the system are located at $i_x = 0$ and $i_x = L$, and we introduce a site-dependent potential

$U(i_x)$ to model the interface barrier. To investigate the model of Eq. (1) we decouple the interaction term in the Hartree-Fock approximation by introducing the pairing amplitude on a bond, $\Delta_{\mathbf{ij}} = \langle c_{\mathbf{i}\uparrow} c_{\mathbf{j}\downarrow} \rangle$, so that $V n_{\mathbf{i}\uparrow} n_{\mathbf{j}\downarrow} \simeq (\Delta_{\mathbf{ij}} c^{\dagger}_{\mathbf{j}\downarrow} c^{\dagger}_{\mathbf{i}\uparrow} + \Delta^{*}_{\mathbf{ij}} c_{\mathbf{i}\uparrow} c_{\mathbf{j}\downarrow} - |\Delta_{\mathbf{ij}}|^2)$. These pairing amplitudes on each bond yield the spin singlet (S) and triplet (T) components, $\Delta^{S,T} = (\Delta_{\mathbf{ij}} \pm \Delta_{\mathbf{ji}})/2$, that define the superconducting order parameters with s- or p-wave symmetry, i.e. $\Delta_s(\mathbf{i}) = (\Delta^S_{\mathbf{i},\mathbf{i}+\hat{\mathrm{x}}} + \Delta^S_{\mathbf{i},\mathbf{i}-\hat{\mathrm{x}}} + \Delta^S_{\mathbf{i},\mathbf{i}+\hat{\mathrm{y}}} + \Delta^S_{\mathbf{i},\mathbf{i}-\hat{\mathrm{y}}})/4$ and $\Delta_{p_{x(y)}}(\mathbf{i}) = (\Delta^T_{\mathbf{i},\mathbf{i}+\hat{\mathrm{x}}(\hat{\mathrm{y}})} - \Delta^T_{\mathbf{i},\mathbf{i}-\hat{\mathrm{x}}(\hat{\mathrm{y}})})/2$, which are then determined self-consistently [9]. Singlet d-wave superconductivity is possible but does not appear in the parameter range where we work [9]. In the bulk ($U = 0$) the most favorable pairing state for this model depends on the electron density, n, and, in particular, the chiral $p_x + ip_y$ order is stabilized in the region between half-filling, $\mu \simeq 0$, and high (low) density ($|\mu| \simeq 2.5$) [10]. Hence, we choose the chemical potential to be $|\mu| \simeq 1.8$, in the window of stability, so that in the absence of $U(i_x)$ the filling is $n \approx 0.4$. All the numerical results below have been obtained for a pairing interaction $V = 2.5$ and a system size $L = 80$, and we checked that greater values of L leave the results qualitatively unchanged. Many studies of the surface states assume a sharp step-like potential at the surface [11]: we find qualitative differences between the results obtained using such assumptions and the behavior of the system using a realistic surface barrier. One very important distinction is that a finite-width barrier changes the electron density near the boundary, thereby enabling the emergence of superconducting components competing with the dominant triplet one.

Numerical results. Fig.1 shows representative results for the electron density and spin polarization, as well as the evolution of the superconducting order parameters for different strength of the surface potential. Here we assumed a rectangular potential barrier of height U (in units of the hopping t) near the left edge of the system, $0 \leq i_x \leq 8$. Finite values of U lead to the depletion of the electron density near the edge, Fig.1(a). For $U = 0$, Fig.1(c), we find the expected result: the interface is pairbreaking for the p_x component of the order parameter, while the p_y component remains essentially constant. However, as U exceeds a critical value, here found to be $U_c \simeq 0.19$, a subdominant s-wave component of the order parameter appears, Fig.1(d)-(f), and there is a substantial region of coexistence of the superconducting order parameters of different parity. Note that mixed parity order parameters are generally allowed here since the presence of the barrier breaks the inversion symmetry of the lattice. A remarkable feature is that the emergence of the mixed-parity phase is accompanied by the appearance of a finite spin polarization in that same region, Fig.1(b). As the barrier becomes higher, fewer carriers remain in the boundary layer, and the magnetization gradually decreases.

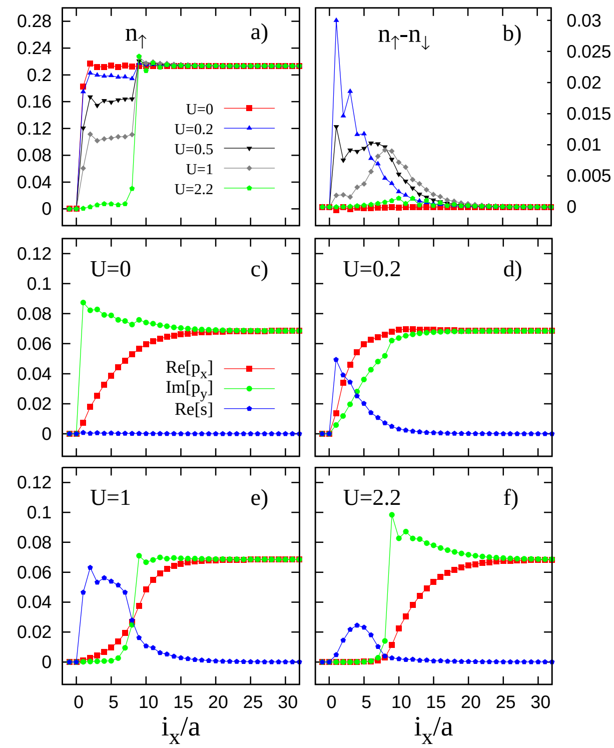

FIG. 1. (color online) Evolution of the electron density and the order parameters with the surface barrier. The s-wave refers to nearest-neighbor pairing. a-b) spin-up electron density and spin polarization for the several values of the barrier height U, c)-f) superconducting order parameters for different heights of the potential barrier U extending from $i_x = 0$ to $i_x = 8$.

Analysis of the energy spectrum $E_n(k_y)$ (due to translational invariance along the interface k_y is a good quantum number) obtained from the numerical solution of the Bogoliubov-De Gennes equations confirms that the local magnetization is due to the gapless edge modes propagating in one direction along the system boundary. This is clear from Fig. 2, where the two originally spin-degenerate chiral edge states associated with the left boundary become split once the barrier potential exceeds $U_c \simeq 0.19$. This splitting occurs concomitantly with the appearance of a spin polarization at that edge (of course, the counterpropagating edge mode associated with the right edge is not affected). As the barrier height is increased the splitting between the spin-up and spin-down modes at the edge decreases, and eventually leads to lower and lower values of the magnetization, as the boundary region becomes depleted. We also notice that extra midgap states appear close the bottom and the top of the gap edge with a structure that evolves from an asymmetric profile in the case of an extended region of singlet-triplet coexistence at the surface, i.e. for $U = 0.2$ and 1.0, to a more symmetric one around $k_y = 0$ for $U = 2.2$.

The implication of this result is that a spin accumulation may occur in a triplet superconductor *without the proximity coupling to an exotic system*. The characteristic length scale over which the magnetization appears in our case is comparable to the width of the region where the density gradient is present: this is because for the present values of parameters the superconducting coherence length is comparable to that width. In general, if the screening of the surface potential occurs on a much shorter scale than the coherence length, the surface barrier nucleates the subdominant s-wave component of the pairing amplitude, and the length scale of the coexistence is set by the coherence length. Note that this situation is quite different from the case discussed in Refs.12–14, where spin polarization appears at the interface separating a triplet and a singlet superconductor only for a non-trivial phase difference. In fact, as we show below, the requirements for the spin accumulation are very different for the two geometries. The physical distinction is that the studies of superconductor-insulator-superconductor (S-I-S) junctions within standard BTK-like techniques [11] use the scattering formulation of the boundary problem between two semi-infinite materials, whereas here the polarization is obtained from a fully self-consistent solution of the Bogoliubov-de Gennes equations in the presence of a realistic boundary potential.

Symmetry analysis. To elucidate the origin of the spin polarization we analyse the problem from the symmetry perspective. The main insight from the numerical results is that the singlet and the triplet components of the order parameter coexist over a finite length scale near the edge due to the extended nature of the boundary potential, and because of the absence of the inversion symmetry near the interface. We first note that in this situation the combined order parameter is non-unitary. In the 2x2 spin space the order parameter is commonly written in the form [15] $\boldsymbol{\Delta}_{\boldsymbol{k}} = i\left[(\boldsymbol{d}_{\boldsymbol{k}}\cdot\boldsymbol{\sigma}) + \psi_{\boldsymbol{k}}\right]\sigma_y$, where σ_i are Pauli matrices, and $\boldsymbol{d}_{\boldsymbol{k}}$ and $\psi_{\boldsymbol{k}}$ are the three triplet and the singlet pairing amplitudes respectively. In that case the gauge-invariant product is given by $\boldsymbol{\Delta}\boldsymbol{\Delta}^{\dagger} = |\boldsymbol{d}_{\boldsymbol{k}}|^2\sigma_0 + |\psi_{\boldsymbol{k}}|^2 + \boldsymbol{q}_{\boldsymbol{k}}\cdot\boldsymbol{\sigma}$ with $\boldsymbol{q}_{\boldsymbol{k}} = \psi_{\boldsymbol{k}}\boldsymbol{d}^{\star}_{\boldsymbol{k}} + \psi^{\star}_{\boldsymbol{k}}\boldsymbol{d}_{\boldsymbol{k}} + i\left[\boldsymbol{d}_{\boldsymbol{k}}\times\boldsymbol{d}^{\star}_{\boldsymbol{k}}\right]$. In our case the bulk triplet superconductor is unitary, $\boldsymbol{d}\|\widehat{\boldsymbol{z}}$ and therefore $\boldsymbol{d}_{\boldsymbol{k}}\times\boldsymbol{d}^{\star}_{\boldsymbol{k}} = 0$. However, in the coexistence region, $\boldsymbol{q}_{\boldsymbol{k}} = 2\mathrm{Re}\left[\psi_{\boldsymbol{k}}\boldsymbol{d}^{\star}_{\boldsymbol{k}}\right] \neq 0$ since, as Fig. 1 shows, the self-consistent solution yields the *in-phase* singlet and triplet p_x components.

Nonvanishing $\boldsymbol{q}_{\boldsymbol{k}}$ vector suggests, but by itself does not necessarily require, a finite spin polarization, since its average over the direction of the momenta $\boldsymbol{k}$ may still vanish (this averaging is difficult to carry out analytically in a system without translation invariance such as our boundary problem). Therefore we consider a Ginzburg-Landau (GL) expansion of the magnetic contribution to the free energy density f_m in the region of coexistence. We choose the direction of the magnetization $\boldsymbol{m}$ parallel to $\boldsymbol{d}(\boldsymbol{r}) = \widehat{\boldsymbol{z}}\left(\eta_x(\boldsymbol{r}) + i\eta_y(\boldsymbol{r})\right)$, along the $\widehat{\boldsymbol{z}}$-axis, as required by the spin rotation invariance, and assume that the pairing amplitudes depend only on the coordinate x normal to the boundary. Then the GL expansion allows for the terms linear in m and the gradient of the p_x-component of the triplet pairing,

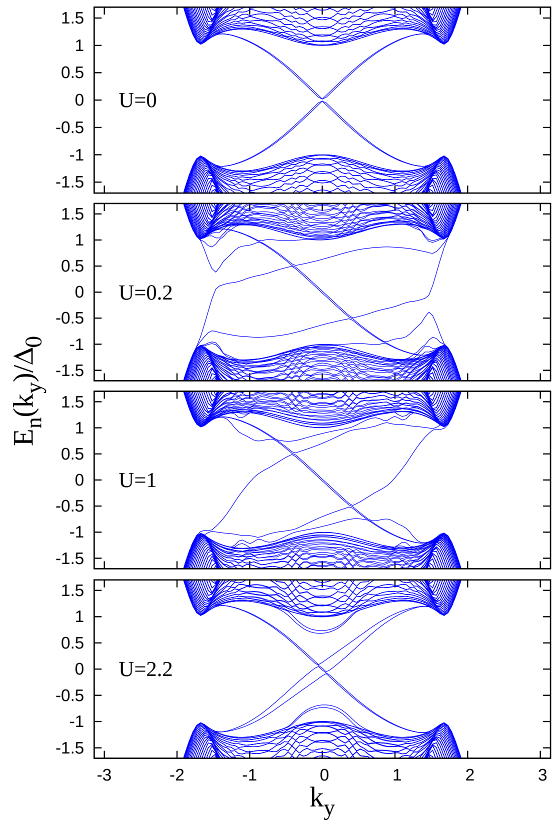

FIG. 2. (color online) Energy spectrum of the solutions of the Bogoliubov-de Gennes equations scaled to the superconducting gap Δ_0 of the homogeneous spin triplet superconductor. Upper panel: pure chiral phase. Two dispersing branches crossing $E = 0$ correspond to the modes along the left and the right edges of the sample. Lower panels: mixed-parity phases. The right edge mode remains unchanged while the modes along the left edge become spin-split. Extra midgap states which are spin-polarized appear at the bottom (occupied) and the top edge (unoccupied) of the gap reflecting the occurrence of a mixed-parity coexisting region. The latter and the spin-split chiral states both contribute to the overall spin accumulation.

$$f_m = m^2 + (\partial_x m)^2 + \alpha m\Big\{\beta\partial_x\left[\eta_x\psi^{\star} + \eta^{\star}_x\psi\right] + \\ + \left[\psi^{\star}(\partial_x\eta_x) + \psi(\partial_x\eta^{\star}_x)\right] - \left[\eta^{\star}_x(\partial_x\psi) + \eta_x(\partial_x\psi^{\star})\right]\Big\}. \tag{2}$$

Since the presence of the linear in m term means that for any values of the coefficients the minimum of the free energy is at finite m, it immediately follows that in the region of the coexistence a finite magnetization appears unless the singlet and the triplet p_x components are out of phase and the product $\eta_x\psi$ is purely imaginary. This

observation emphatically brings forth the distinction between our results and those for the S-I-S junction [12–14], where the spin accumulation only occurs if the two pairing components are out of phase, the exact opposite of the result we find.

Only the p_x-component of the triplet appears in the GL expansion above; in principle the term $\partial_y \eta_y$ is also allowed by symmetry [16], but does not appear under the assumption of the translational invariance along the interface. It follows that the time-reversal symmetry breaking by the bulk chiral triplet state is not at the origin of the magnetization of the Andreev bound states: the same result would be achieved for purely real p_x bulk triplet superconductivity, while for the imaginary p_x bulk pairing with real subdominant s-wave pairing near the interface no magnetization appears. To explore this connection, we consider a situation when in proximity of the left edge ($0 < i_x < \bar{i}_x$, with $\bar{i}_x = 10$) a purely local s-wave potential is the only source of pairing, with V still effective in the remaining part of the system, and use as input a real s-wave order parameter for $0 < i_x \leq \bar{i}_x$ and a purely imaginary p_x-wave one for $i_x > \bar{i}_x$. Working at the same electron density as before (with $U = 0$), and without the self-consistent iterative procedure (which would unavoidably lead to a mixing of real and imaginary components), we see from the panels a) and c) of Fig.3 that, in spite of the parity mixing occurring around $i_x = \bar{i}_x$, no appreciable spin polarization is observed. On the other hand, when in the same configuration one uses for $i_x > \bar{i}_x$ a purely real p_x input order parameter to generate a non-unitary mixed phase around $i_x = \bar{i}_x$, a significant magnetization clearly develops in the mixing region. This is exhibited in the panels b) and d) of Fig. 3, and supports our conclusion based on symmetry arguments.

Discussion. We show that Andreev bound states near a boundary of a triplet superconductor can be spin-polarized. The origin of the spin polarization is in the emergence of the coexistence regime of the triplet and the subdominant singlet pairing components near the interface. Our numerical results demonstrate that the two are phase-locked, and both the numerical fully self-consistent solution of the Bogoliubov-de Gennes equations and the Ginzburg-Landau analysis indicates that magnetization inevitably appears when the two order parameters lead to a non-unitary configuration and are spatially varying. We find that the symmetry-breaking at the surface is unrelated to the chiral nature of the bulk superconducting state, and therefore may be expected in a much wider class of triplet superconductors. It would also be very interesting to check whether similar effects occur at the interfaces involving non-centrosymmetric superconductors, where the singlet and the triplet components are intrinsically mixed in the bulk yielding measurable spin effects at the interface [17–20], as well as in the proximity structures with topological materials. We leave this for future investigations.

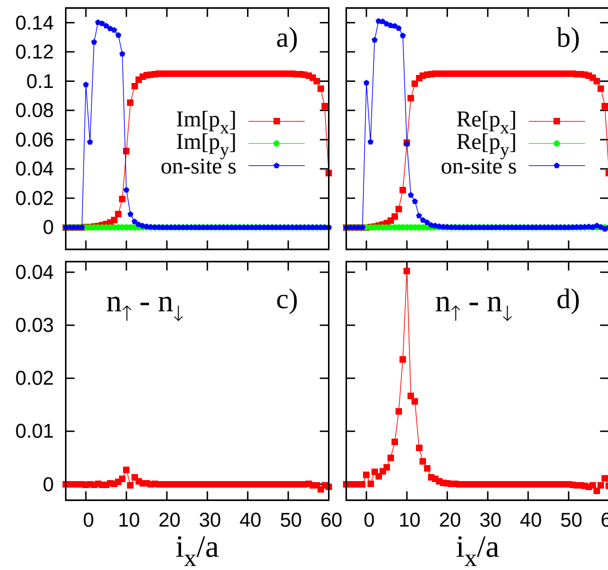

FIG. 3. (color online) Spatial evolution of singlet and triplet order parameters and of the magnetization in the case of unitary, a) and c), and non-unitary states, b) and d), respectively, as realized in a thin vertical slab of the system around the point ($i_x = 10$). A real spin singlet on-site pairing amplitude and a purely real or a purely imaginary triplet pairing amplitude are assumed in input ($i_x < 10$ and $i_x > 10$, respectively).

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